



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:53 am BST

PDB ID : 1Q7Q
Title : Cobalamin-dependent methionine synthase (1-566) from *T. maritima* (Oxidized, Orthorhombic)
Authors : Evans, J.C.; Huddler, D.P.; Hilgers, M.T.; Romanchuk, G.; Matthews, R.G.; Ludwig, M.L.
Deposited on : 2003-08-19
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

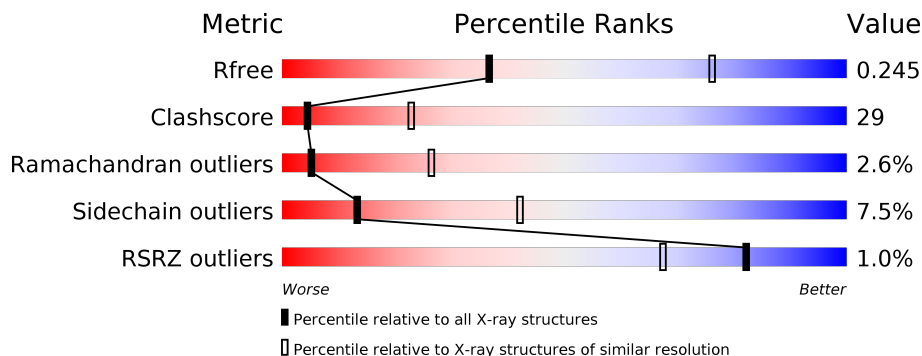
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	566	<div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 15px; border: 1px solid black; position: relative;"> <div style="width: 52%; height: 100%; background-color: green;"></div> <div style="width: 42%; height: 100%; background-color: yellow;"></div> <div style="width: 5%; height: 100%; background-color: orange;"></div> </div> <div style="margin-left: 5px;">%</div> </div> <p style="text-align: center;">52% 42% 5%</p>
1	B	566	<div style="display: flex; align-items: center;"> <div style="width: 10px; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 100%; height: 15px; border: 1px solid black; position: relative;"> <div style="width: 49%; height: 100%; background-color: green;"></div> <div style="width: 42%; height: 100%; background-color: yellow;"></div> <div style="width: 6%; height: 100%; background-color: orange;"></div> <div style="width: 3%; height: 100%; background-color: grey;"></div> </div> <div style="margin-left: 5px;">%</div> </div> <p style="text-align: center;">49% 42% 6% ..</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9031 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 5-methyltetrahydrofolate S-homocysteine methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	565	4467	2866	747	841	13	0	0	0
1	B	552	4370	2805	731	821	13	0	0	0

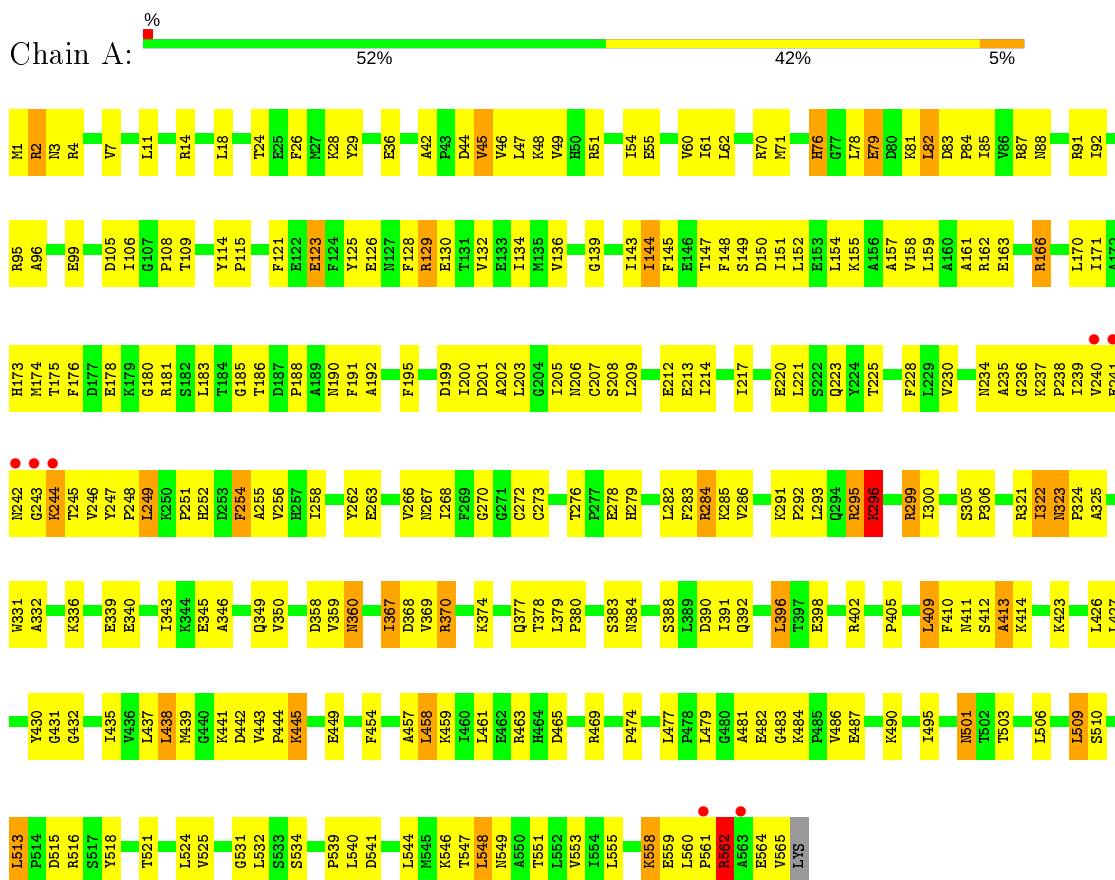
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	103	103	103	0	0
2	B	91	91	91	0	0

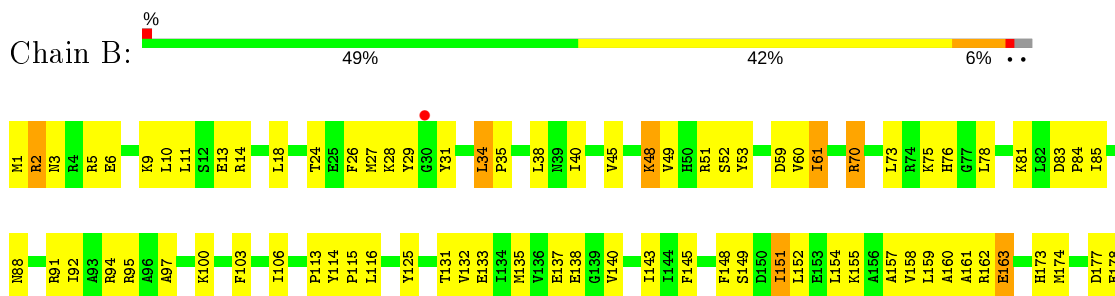
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 5-methyltetrahydrofolate S-homocysteine methyltransferase



- Molecule 1: 5-methyltetrahydrofolate S-homocysteine methyltransferase



K179	G180	R181	S182	L183	P188	F191	A192	I193	L198	D199	I200	D201	A202	L203	G204	L205	I206	C207	S208	L209	G210	P211	E212	E213	I214	L215	P216	I217	F218	Q219	E220	L221	S222	Q223	K227	F228	L229	V230	M234	A235	P236	I239	V240	E241	I242	G243	K244	T245	V246	Y247	P248	L249	K250
P251	E252	D253	F254	A255	V256	H257	I258	D259	S260	Y261	Y262	E263	V266	M267	I268	F269	G270	G271	C272	G273	R274	T275	E278	H279	V280	K281	L282	K285	V286	R290	L293	Q294	R295	K296	I300	P306	E320	R321	I322	N323	P324	K329	L330	W331	A332	F333	M334	N338	E339				
E340	I341	V342	I343	K344	E345	A346	K347	T348	Q349	V350	E351	L357	N360	F361	G362	I363	E364	V369	R370	Y371	V372	I375	V280	L379	P380	P386	L387	S388	Q392	N393	L396	T397	E398	R399	A400	L401	R402	A403	Y404	P405	S408	L409	F410	N411	S412	A413	D416	E417	E418	E419			
I420	E421	M422	K423	I424	H425	L426	L427	Y430	L434	I435	M439	G440	K441	D442	V443	P444	K445	E448	E449	R450	K451	E452	Y453	F454	E455	L458	K459	I460	L461	E462	R463	H464	S467	V470	I471	P474	L479	G480	A481	E482	G483	K484	P485	V486	E487	V488	L489	K490	T491	I492			
E493	F494	T503	L506	S507	M508	L509	SER	PHE	GLY	LEU	PRO	ASP	R516	S517	Y518	T521	A522	F523	L524	V525	I528	S529	K530	Q531	L532	I536	M537	M538	P539	L540	P541	E542	L548	T551	I554	L555	K558	LEU	PRO	ARG	ALA	GLU	VAL	LYS									

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.58Å 169.02Å 174.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 46.39 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 90.6 (46.39-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 3.12Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.265 0.204 , 0.245	Depositor DCC
R_{free} test set	4583 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtrriage
Anisotropy	0.340	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 73.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.031 for -h,l,k	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9031	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/4550	0.66	0/6145
1	B	0.41	0/4449	0.66	0/6005
All	All	0.40	0/8999	0.66	0/12150

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4467	0	4553	254	0
1	B	4370	0	4467	257	0
2	A	103	0	0	26	0
2	B	91	0	0	7	0
All	All	9031	0	9020	510	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (510) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ASP:O	1:B:263:GLU:HG2	1.64	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ARG:HH21	1:A:166:ARG:HB2	1.29	0.93
1:A:296:LYS:NZ	1:A:296:LYS:HA	1.89	0.87
1:B:271:GLY:HA3	1:B:275:THR:HG21	1.57	0.86
1:A:54:ILE:HD11	1:A:61:ILE:HD13	1.57	0.86
1:B:372:VAL:HG11	1:B:396:LEU:HD11	1.59	0.84
1:A:558:LYS:HG3	1:A:559:GLU:N	1.91	0.83
1:B:455:GLU:O	1:B:459:LYS:HG3	1.79	0.82
1:B:439:MET:HG2	1:B:440:GLY:H	1.44	0.82
1:A:444:PRO:HB3	1:A:449:GLU:HG2	1.62	0.82
1:A:242:ASN:HB2	1:A:244:LYS:HE3	1.60	0.81
1:A:70:ARG:HB3	2:A:636:HOH:O	1.80	0.81
1:B:479:LEU:HA	1:B:483:GLY:HA2	1.63	0.81
1:A:284:ARG:HA	1:A:284:ARG:HE	1.46	0.80
1:A:151:ILE:HD11	1:A:306:PRO:HA	1.63	0.80
1:B:230:VAL:HG22	1:B:268:ILE:HB	1.64	0.79
1:B:151:ILE:HD11	1:B:306:PRO:HG3	1.64	0.79
1:A:209:LEU:HB2	1:A:214:ILE:HG12	1.64	0.78
1:A:390:ASP:HA	2:A:574:HOH:O	1.83	0.76
1:A:54:ILE:HD13	1:A:96:ALA:O	1.85	0.76
1:A:114:TYR:CD1	1:A:115:PRO:HA	2.21	0.76
1:A:515:ASP:HB3	1:A:518:TYR:HD1	1.52	0.75
1:B:409:LEU:HD21	1:B:435:ILE:HD11	1.68	0.74
1:B:370:ARG:HB2	1:B:370:ARG:HH21	1.52	0.73
1:A:402:ARG:HG2	1:A:430:TYR:CE1	2.23	0.73
1:A:171:ILE:HG12	1:A:202:ALA:HB3	1.69	0.73
1:A:166:ARG:HB2	1:A:166:ARG:NH2	2.03	0.73
1:A:244:LYS:HG3	1:A:245:THR:H	1.54	0.73
1:A:360:ASN:HB2	1:A:390:ASP:HB3	1.68	0.72
1:A:562:ARG:CZ	1:A:562:ARG:HA	2.19	0.72
1:A:212:GLU:HG2	2:A:624:HOH:O	1.88	0.72
1:B:435:ILE:HD13	1:B:471:ILE:HG12	1.71	0.72
1:B:364:GLU:OE2	1:B:392:GLN:HG2	1.89	0.71
1:A:213:GLU:HG2	2:A:630:HOH:O	1.90	0.71
1:B:29:TYR:CE1	1:B:48:LYS:HD3	2.26	0.70
1:B:244:LYS:HA	1:B:244:LYS:NZ	2.06	0.70
1:A:1:MET:HG3	1:A:139:GLY:HA3	1.72	0.70
1:A:445:LYS:H	1:A:445:LYS:HD2	1.57	0.70
1:B:1:MET:HG3	1:B:140:VAL:O	1.92	0.69
1:B:439:MET:CG	1:B:440:GLY:H	2.03	0.69
1:A:255:ALA:O	1:A:286:VAL:HG11	1.92	0.69
1:A:296:LYS:HZ3	1:A:296:LYS:HA	1.56	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:GLU:HB3	1:B:536:ILE:HG22	1.74	0.69
1:B:132:VAL:HG13	1:B:143:ILE:CD1	2.22	0.69
1:A:411:ASN:HB3	2:A:574:HOH:O	1.92	0.69
1:A:18:LEU:HD23	1:A:60:VAL:HG13	1.75	0.68
1:A:4:ARG:HD3	1:A:201:ASP:OD2	1.94	0.68
1:A:482:GLU:HB3	1:A:484:LYS:HE3	1.74	0.68
1:A:180:GLY:O	1:A:188:PRO:HD3	1.94	0.68
1:B:324:PRO:HG2	1:B:362:GLY:N	2.09	0.67
1:B:151:ILE:H	1:B:151:ILE:HD13	1.59	0.67
1:A:549:ASN:O	1:A:553:VAL:HG23	1.93	0.67
1:B:244:LYS:HZ3	1:B:244:LYS:HA	1.59	0.67
1:B:244:LYS:HZ2	1:B:245:THR:H	1.43	0.67
1:A:299:ARG:HD2	1:A:300:ILE:N	2.10	0.66
1:B:479:LEU:HD22	1:B:509:LEU:HG	1.77	0.66
1:B:537:MET:HE1	1:B:548:LEU:HD22	1.78	0.66
1:A:562:ARG:HA	1:A:562:ARG:NE	2.10	0.66
1:A:128:PHE:O	1:A:132:VAL:HG23	1.96	0.66
1:A:145:PHE:CE2	1:A:157:ALA:HB1	2.31	0.65
1:B:3:ASN:OD1	1:B:6:GLU:HG3	1.96	0.65
1:A:515:ASP:HB3	1:A:518:TYR:CD1	2.31	0.65
1:A:285:LYS:HA	2:A:658:HOH:O	1.95	0.65
1:B:463:ARG:HH21	1:B:463:ARG:HB2	1.62	0.65
1:A:442:ASP:HB3	2:A:587:HOH:O	1.95	0.65
1:B:364:GLU:CD	1:B:392:GLN:HG2	2.17	0.65
1:A:132:VAL:HG11	1:A:161:ALA:HA	1.79	0.64
1:A:87:ARG:O	1:A:91:ARG:HG3	1.97	0.64
1:A:42:ALA:O	1:A:45:VAL:HG23	1.97	0.64
1:B:463:ARG:HB2	1:B:463:ARG:NH2	2.12	0.64
1:A:132:VAL:O	1:A:136:VAL:HG23	1.98	0.64
1:B:202:ALA:HB2	1:B:228:PHE:HB2	1.79	0.64
1:B:133:GLU:O	1:B:137:GLU:HG3	1.97	0.63
1:A:132:VAL:HG13	1:A:143:ILE:HD13	1.80	0.63
1:B:9:LYS:O	1:B:13:GLU:HG3	1.98	0.63
1:B:370:ARG:HB2	1:B:370:ARG:NH2	2.13	0.63
1:B:48:LYS:HE2	1:B:48:LYS:C	2.19	0.63
1:A:79:GLU:HB3	2:A:577:HOH:O	1.99	0.63
1:A:88:ASN:O	1:A:92:ILE:HG12	1.99	0.63
1:B:471:ILE:HD11	1:B:503:THR:HB	1.81	0.63
1:B:49:VAL:O	1:B:52:SER:HB3	1.99	0.63
1:B:320:GLU:HB3	1:B:536:ILE:CG2	2.29	0.63
1:B:296:LYS:HA	1:B:296:LYS:HE3	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ASP:CB	2:A:587:HOH:O	2.48	0.62
1:B:238:PRO:O	1:B:239:ILE:HB	2.00	0.62
1:B:402:ARG:HB3	1:B:430:TYR:CE1	2.35	0.62
1:B:540:LEU:HD12	1:B:540:LEU:N	2.14	0.62
1:A:564:GLU:HG2	1:A:565:VAL:N	2.15	0.61
1:B:439:MET:HG2	1:B:440:GLY:N	2.14	0.61
1:B:18:LEU:CD1	1:B:60:VAL:HB	2.30	0.61
1:A:132:VAL:HG13	1:A:143:ILE:CD1	2.31	0.61
1:A:291:LYS:HG3	1:A:292:PRO:HD2	1.81	0.61
1:A:29:TYR:CE2	1:A:48:LYS:HD2	2.35	0.61
1:A:558:LYS:HG3	1:A:559:GLU:H	1.65	0.61
1:B:539:PRO:HG2	1:B:540:LEU:HD12	1.83	0.61
1:A:81:LYS:O	1:A:85:ILE:HG12	2.00	0.61
1:B:106:ILE:HD11	1:B:135:MET:SD	2.41	0.61
1:A:346:ALA:O	1:A:350:VAL:HG23	2.01	0.60
1:A:295:ARG:HH21	1:A:295:ARG:HG2	1.67	0.60
1:A:521:THR:O	1:A:525:VAL:HG23	2.02	0.60
1:A:108:PRO:HB2	2:A:661:HOH:O	2.01	0.60
1:A:70:ARG:NE	2:A:636:HOH:O	2.35	0.60
1:B:349:GLN:HB2	1:B:357:LEU:HD21	1.83	0.60
1:A:186:THR:HA	2:A:609:HOH:O	2.01	0.59
1:B:106:ILE:HD12	1:B:131:THR:HG21	1.83	0.59
1:B:372:VAL:HG11	1:B:396:LEU:CD1	2.29	0.59
1:B:70:ARG:HH21	1:B:70:ARG:HG3	1.67	0.59
1:B:440:GLY:O	1:B:442:ASP:N	2.35	0.59
1:B:445:LYS:HG2	1:B:482:GLU:OE1	2.02	0.59
1:A:174:MET:HG3	1:A:191:PHE:CE1	2.37	0.59
1:B:2:ARG:HD3	1:B:2:ARG:N	2.16	0.59
1:A:145:PHE:HB3	1:A:148:PHE:CE1	2.37	0.59
1:A:178:GLU:HG2	2:A:666:HOH:O	2.03	0.59
1:A:479:LEU:HG	1:A:509:LEU:HD22	1.84	0.59
1:B:88:ASN:O	1:B:92:ILE:HG13	2.02	0.58
1:A:565:VAL:O	1:A:565:VAL:HG13	2.03	0.58
1:A:438:LEU:HD12	1:A:474:PRO:HA	1.85	0.58
1:A:360:ASN:CB	1:A:390:ASP:HB3	2.34	0.58
1:B:479:LEU:CD2	1:B:479:LEU:H	2.16	0.58
1:B:320:GLU:HG3	1:B:537:MET:O	2.04	0.58
1:A:162:ARG:NH1	1:A:170:LEU:HB2	2.18	0.58
1:B:444:PRO:HD3	1:B:453:TYR:HE1	1.68	0.58
1:A:166:ARG:HH21	1:A:166:ARG:CB	2.09	0.57
1:A:147:THR:HG22	1:A:147:THR:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:ASP:O	1:B:443:VAL:HG23	2.02	0.57
1:B:27:MET:HE3	2:B:639:HOH:O	2.03	0.57
1:A:345:GLU:O	1:A:349:GLN:HG3	2.05	0.57
1:A:252:HIS:O	1:A:256:VAL:HG13	2.05	0.57
1:A:99:GLU:OE1	1:A:99:GLU:HA	2.03	0.57
1:A:70:ARG:HD3	1:A:130:GLU:CD	2.24	0.57
1:B:209:LEU:HB2	1:B:214:ILE:CD1	2.34	0.57
1:A:483:GLY:O	1:A:484:LYS:HD2	2.04	0.57
1:B:243:GLY:O	1:B:244:LYS:O	2.22	0.57
1:A:207:CYS:O	1:A:208:SER:HB2	2.05	0.57
1:B:439:MET:CG	1:B:440:GLY:N	2.68	0.57
1:B:412:SER:H	1:B:435:ILE:HB	1.69	0.56
1:B:26:PHE:O	1:B:31:TYR:HB2	2.06	0.56
1:A:276:THR:HG22	2:A:589:HOH:O	2.05	0.56
1:B:479:LEU:HA	1:B:483:GLY:CA	2.36	0.56
1:B:341:ILE:HG23	1:B:342:VAL:N	2.21	0.56
1:B:435:ILE:CD1	1:B:471:ILE:HG12	2.34	0.56
1:A:551:THR:HG22	1:A:555:LEU:HD12	1.88	0.56
1:A:3:ASN:O	1:A:7:VAL:HG23	2.06	0.56
1:A:192:ALA:HB2	1:A:221:LEU:HD12	1.86	0.56
1:B:205:ILE:HD13	1:B:217:ILE:HG22	1.87	0.56
1:B:125:TYR:CE1	1:B:160:ALA:HA	2.41	0.55
1:A:370:ARG:NH2	1:A:370:ARG:HB2	2.20	0.55
1:A:441:LYS:HG3	2:A:571:HOH:O	2.05	0.55
1:A:92:ILE:O	1:A:95:ARG:HB2	2.06	0.55
1:A:209:LEU:HB2	1:A:214:ILE:CG1	2.35	0.55
1:B:484:LYS:N	1:B:485:PRO:HD3	2.21	0.55
1:B:155:LYS:O	1:B:159:LEU:HB2	2.06	0.55
1:A:251:PRO:O	1:A:282:LEU:HD22	2.07	0.55
1:A:4:ARG:NH1	1:A:162:ARG:CZ	2.69	0.55
1:B:295:ARG:HH21	1:B:295:ARG:HG3	1.72	0.55
1:B:29:TYR:HE1	1:B:48:LYS:HD3	1.71	0.55
1:A:332:ALA:O	1:A:336:LYS:HG3	2.07	0.55
1:B:252:HIS:O	1:B:256:VAL:HG13	2.07	0.54
1:B:18:LEU:HD12	1:B:60:VAL:HB	1.88	0.54
1:B:209:LEU:HB3	1:B:213:GLU:HB2	1.89	0.54
1:B:114:TYR:CD1	1:B:115:PRO:HA	2.43	0.54
1:A:121:PHE:HZ	1:A:159:LEU:HD12	1.73	0.54
1:A:162:ARG:NH1	1:A:170:LEU:HD12	2.22	0.54
1:B:3:ASN:OD1	1:B:5:ARG:HB2	2.08	0.54
1:A:513:LEU:O	1:A:516:ARG:HG2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:GLU:HG2	1:B:464:HIS:NE2	2.23	0.54
1:B:192:ALA:HB2	1:B:221:LEU:HD12	1.90	0.53
1:B:95:ARG:HH11	1:B:95:ARG:HG2	1.72	0.53
1:A:266:VAL:HG22	1:A:267:ASN:N	2.23	0.53
1:A:398:GLU:HG3	1:A:426:LEU:HD22	1.90	0.53
1:A:438:LEU:HD11	1:A:495:ILE:HD11	1.91	0.53
1:A:176:PHE:CE1	1:A:205:ILE:HD12	2.44	0.53
1:B:208:SER:H	1:B:234:ASN:HD21	1.57	0.53
1:B:416:ASP:O	1:B:418:GLU:N	2.41	0.53
1:B:458:LEU:O	1:B:462:GLU:HB2	2.07	0.53
1:A:151:ILE:HG22	1:A:195:PHE:HE1	1.74	0.53
1:A:358:ASP:HA	1:A:388:SER:HB3	1.90	0.53
1:B:474:PRO:HD2	1:B:503:THR:O	2.09	0.53
1:B:551:THR:HG22	1:B:555:LEU:CD2	2.38	0.53
1:A:321:ARG:HD2	1:A:540:LEU:HD22	1.90	0.53
1:A:151:ILE:O	1:A:155:LYS:HB2	2.08	0.53
1:A:240:VAL:HG23	1:A:240:VAL:O	2.09	0.53
1:A:383:SER:O	1:A:384:ASN:HB2	2.09	0.53
1:B:413:ALA:HB2	1:B:434:LEU:HD11	1.91	0.53
1:A:235:ALA:HB3	1:A:247:TYR:HB3	1.90	0.53
1:A:284:ARG:CA	1:A:284:ARG:HE	2.18	0.53
1:B:191:PHE:CZ	1:B:203:LEU:HD12	2.44	0.53
1:B:404:TYR:CD1	1:B:408:SER:HB3	2.44	0.53
1:A:251:PRO:HB3	1:A:282:LEU:HD13	1.90	0.52
1:B:61:ILE:HD11	1:B:97:ALA:HB2	1.91	0.52
1:A:202:ALA:HB2	1:A:228:PHE:HB2	1.91	0.52
1:A:296:LYS:HZ2	1:A:296:LYS:HA	1.69	0.52
1:A:126:GLU:OE1	1:A:129:ARG:NH1	2.42	0.52
1:A:345:GLU:HG2	2:A:651:HOH:O	2.08	0.52
1:B:282:LEU:O	1:B:282:LEU:HD23	2.09	0.52
1:B:173:HIS:CD2	1:B:204:GLY:HA3	2.44	0.52
1:B:479:LEU:HD23	1:B:479:LEU:H	1.74	0.52
1:B:524:LEU:O	1:B:528:ILE:HG13	2.09	0.52
1:A:151:ILE:HD11	1:A:306:PRO:CA	2.36	0.52
1:A:151:ILE:HG22	1:A:195:PHE:CE1	2.45	0.52
1:B:538:ASN:OD1	1:B:540:LEU:HB2	2.10	0.52
1:B:14:ARG:HA	1:B:290:ARG:O	2.08	0.52
1:B:106:ILE:O	1:B:145:PHE:HA	2.10	0.52
1:B:81:LYS:C	1:B:84:PRO:HD2	2.30	0.52
1:A:176:PHE:HE1	1:A:205:ILE:HD12	1.75	0.52
1:B:508:ASN:O	1:B:509:LEU:HD13	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:THR:HG22	1:B:555:LEU:HD23	1.92	0.51
1:A:212:GLU:HB3	1:A:213:GLU:OE2	2.10	0.51
1:A:411:ASN:O	1:A:412:SER:HB2	2.09	0.51
1:B:479:LEU:N	1:B:479:LEU:HD23	2.26	0.51
1:A:11:LEU:HD21	1:A:268:ILE:HD11	1.91	0.51
1:A:188:PRO:HB2	1:A:220:GLU:HB3	1.92	0.51
1:A:487:GLU:OE1	1:A:487:GLU:HA	2.11	0.51
1:A:46:VAL:HG12	1:A:92:ILE:HG21	1.91	0.51
1:B:422:MET:HE3	1:B:426:LEU:HD12	1.91	0.51
1:A:62:LEU:HD22	1:A:144:ILE:HG21	1.93	0.51
1:B:131:THR:O	1:B:135:MET:HG3	2.11	0.51
1:B:18:LEU:HB3	1:B:270:GLY:HA3	1.93	0.51
1:B:31:TYR:CE2	1:B:45:VAL:HG21	2.45	0.51
1:B:83:ASP:HB3	1:B:84:PRO:HD3	1.92	0.51
1:A:262:TYR:O	1:A:293:LEU:HD22	2.11	0.51
1:B:213:GLU:O	1:B:216:PRO:HD2	2.11	0.51
1:A:282:LEU:O	1:A:285:LYS:N	2.43	0.51
1:A:410:PHE:HE2	1:A:423:LYS:HD2	1.75	0.51
1:B:205:ILE:CD1	1:B:217:ILE:HG22	2.41	0.51
1:A:439:MET:O	1:A:439:MET:HG3	2.11	0.51
1:A:539:PRO:HG2	1:A:540:LEU:HD12	1.93	0.51
1:B:125:TYR:OH	1:B:163:GLU:HG2	2.11	0.51
1:A:379:LEU:HB2	1:A:380:PRO:HD3	1.92	0.50
1:A:323:ASN:O	1:A:323:ASN:CG	2.49	0.50
1:A:241:GLU:HB2	1:A:246:VAL:HG21	1.92	0.50
1:A:70:ARG:HG2	2:A:578:HOH:O	2.12	0.50
1:A:510:SER:HA	1:A:513:LEU:HD21	1.94	0.50
1:B:480:GLY:O	1:B:481:ALA:HB2	2.12	0.50
1:B:441:LYS:HE3	1:B:453:TYR:HE2	1.76	0.50
1:B:48:LYS:HE2	1:B:49:VAL:N	2.26	0.50
1:B:521:THR:O	1:B:525:VAL:HG23	2.11	0.50
1:B:91:ARG:NE	1:B:138:GLU:OE2	2.44	0.50
1:B:324:PRO:HB3	1:B:331:TRP:HE3	1.75	0.50
1:A:251:PRO:C	1:A:282:LEU:HD22	2.31	0.50
1:A:62:LEU:HB3	1:A:105:ASP:HB2	1.94	0.50
1:B:322:ILE:HG22	1:B:322:ILE:O	2.11	0.50
1:B:467:SER:O	1:B:470:VAL:HG22	2.11	0.50
1:B:492:ILE:HD12	1:B:532:LEU:HD13	1.93	0.50
1:A:378:THR:HG22	1:A:379:LEU:N	2.27	0.50
1:A:391:ILE:HG21	1:A:396:LEU:HB3	1.94	0.50
1:A:292:PRO:HA	2:A:602:HOH:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ARG:HH21	1:A:321:ARG:HG2	1.77	0.50
1:B:34:LEU:HD11	1:B:76:HIS:CD2	2.47	0.50
1:B:479:LEU:HD22	1:B:509:LEU:CG	2.41	0.49
1:A:149:SER:HB3	1:A:183:LEU:HB3	1.94	0.49
1:B:238:PRO:O	1:B:239:ILE:CB	2.60	0.49
1:A:158:VAL:HG23	1:A:159:LEU:N	2.26	0.49
1:A:244:LYS:O	1:A:245:THR:HG23	2.12	0.49
1:A:263:GLU:HA	1:A:293:LEU:CD2	2.42	0.49
1:B:338:ASN:HD22	1:B:339:GLU:H	1.59	0.49
1:B:200:ILE:HD13	1:B:200:ILE:H	1.75	0.49
1:A:487:GLU:OE1	1:A:490:LYS:HD3	2.12	0.49
1:A:95:ARG:HD2	2:A:569:HOH:O	2.11	0.49
1:B:149:SER:HB3	1:B:183:LEU:HB3	1.93	0.49
1:B:331:TRP:HH2	1:B:363:ILE:O	1.96	0.49
1:A:295:ARG:NH2	1:A:295:ARG:HG2	2.26	0.49
1:B:486:VAL:HG22	1:B:490:LYS:HZ2	1.78	0.49
1:A:188:PRO:CG	1:A:217:ILE:HG23	2.43	0.49
1:B:427:LEU:CD1	1:B:434:LEU:HB2	2.43	0.49
1:B:151:ILE:HD11	1:B:306:PRO:CG	2.39	0.49
1:A:306:PRO:HG3	1:A:405:PRO:HB2	1.94	0.48
1:A:409:LEU:HD22	1:A:435:ILE:HG13	1.95	0.48
1:B:259:ASP:O	1:B:263:GLU:CG	2.49	0.48
1:B:422:MET:HE2	1:B:423:LYS:HG3	1.95	0.48
1:B:528:ILE:HD11	1:B:548:LEU:CD1	2.43	0.48
1:B:70:ARG:HH21	1:B:70:ARG:CG	2.25	0.48
1:A:130:GLU:O	1:A:134:ILE:HG12	2.13	0.48
1:A:486:VAL:O	1:A:490:LYS:HG3	2.13	0.48
1:B:207:CYS:HG	1:B:272:CYS:HG	1.60	0.48
1:B:410:PHE:HE2	1:B:423:LYS:HD3	1.78	0.48
1:A:295:ARG:HG3	2:A:659:HOH:O	2.11	0.48
1:A:47:LEU:HD12	1:A:96:ALA:HB2	1.94	0.48
1:A:36:GLU:O	1:A:85:ILE:HG23	2.13	0.48
1:B:211:PRO:HG3	1:B:254:PHE:CE1	2.48	0.48
1:B:420:LEU:C	1:B:424:ILE:HD13	2.34	0.48
1:A:255:ALA:O	1:A:258:ILE:HD13	2.14	0.48
1:A:255:ALA:HB1	1:A:286:VAL:HG21	1.96	0.48
1:A:561:PRO:O	1:A:562:ARG:HB2	2.14	0.48
1:A:114:TYR:HE2	1:A:374:LYS:HZ1	1.55	0.48
1:B:338:ASN:ND2	1:B:339:GLU:N	2.61	0.48
1:B:3:ASN:CG	1:B:5:ARG:HD3	2.34	0.48
1:B:489:LEU:HD21	1:B:523:PHE:CE1	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:GLY:O	1:A:469:ARG:NH2	2.45	0.48
1:B:211:PRO:HD3	1:B:234:ASN:O	2.14	0.48
1:B:238:PRO:O	1:B:246:VAL:O	2.32	0.48
1:B:321:ARG:HG3	1:B:540:LEU:HD13	1.95	0.48
1:A:155:LYS:O	1:A:159:LEU:HG	2.14	0.48
1:A:45:VAL:O	1:A:49:VAL:HG23	2.13	0.48
1:A:46:VAL:CG1	1:A:92:ILE:HG21	2.43	0.48
1:B:486:VAL:HG22	1:B:490:LYS:NZ	2.29	0.48
1:A:186:THR:HG23	1:A:190:ASN:HB3	1.94	0.47
1:A:521:THR:CG2	1:A:547:THR:HG21	2.44	0.47
1:A:54:ILE:HD13	1:A:96:ALA:C	2.34	0.47
1:B:306:PRO:HD3	1:B:405:PRO:O	2.14	0.47
1:B:379:LEU:HB2	1:B:380:PRO:HD3	1.96	0.47
1:A:454:PHE:CE2	1:A:458:LEU:HD12	2.50	0.47
1:B:402:ARG:HB3	1:B:430:TYR:CD1	2.48	0.47
1:A:221:LEU:O	1:A:225:THR:HG22	2.14	0.47
1:A:237:LYS:HE3	2:A:630:HOH:O	2.14	0.47
1:A:114:TYR:CE2	1:A:374:LYS:NZ	2.75	0.47
1:A:414:LYS:HB3	1:A:439:MET:O	2.15	0.47
1:A:560:LEU:HA	1:A:561:PRO:HD3	1.56	0.47
1:B:420:LEU:HD12	1:B:460:ILE:HD12	1.97	0.47
1:A:564:GLU:HG2	1:A:565:VAL:H	1.79	0.47
1:A:200:ILE:CD1	1:A:203:LEU:HD21	2.44	0.47
1:A:321:ARG:HD2	1:A:540:LEU:HD13	1.95	0.47
1:A:244:LYS:HG3	1:A:245:THR:N	2.28	0.47
1:A:427:LEU:O	1:A:431:GLY:N	2.46	0.47
1:B:324:PRO:HB3	1:B:331:TRP:CE3	2.50	0.47
1:B:338:ASN:HD22	1:B:339:GLU:N	2.12	0.47
1:A:444:PRO:CB	1:A:449:GLU:HG2	2.39	0.47
1:B:445:LYS:HB2	1:B:449:GLU:OE2	2.15	0.47
1:A:324:PRO:O	1:A:331:TRP:HB2	2.15	0.46
1:A:564:GLU:O	1:A:565:VAL:HG12	2.15	0.46
1:B:145:PHE:HB3	1:B:148:PHE:CE1	2.49	0.46
1:B:29:TYR:N	1:B:29:TYR:HD2	2.13	0.46
1:B:558:LYS:HB2	2:B:641:HOH:O	2.15	0.46
1:A:412:SER:O	1:A:413:ALA:HB2	2.14	0.46
1:B:188:PRO:HG3	1:B:217:ILE:HG23	1.97	0.46
1:B:222:SER:HB3	1:B:229:LEU:CD1	2.45	0.46
1:A:208:SER:O	1:A:209:LEU:HD23	2.15	0.46
1:A:150:ASP:OD2	1:A:152:LEU:HB3	2.14	0.46
1:A:151:ILE:CD1	1:A:306:PRO:HA	2.39	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ILE:HG22	1:A:392:GLN:N	2.31	0.46
1:B:60:VAL:HG11	1:B:103:PHE:CD2	2.50	0.46
1:A:321:ARG:O	1:A:323:ASN:N	2.49	0.46
1:A:551:THR:HG22	1:A:555:LEU:CD1	2.45	0.46
1:A:228:PHE:HD2	1:A:267:ASN:ND2	2.13	0.46
1:A:441:LYS:NZ	1:A:441:LYS:HB3	2.31	0.46
1:A:81:LYS:O	1:A:85:ILE:CG1	2.63	0.46
1:A:546:LYS:HD2	1:B:518:TYR:CZ	2.51	0.46
1:A:239:ILE:HG13	1:A:248:PRO:HD3	1.98	0.46
1:A:155:LYS:O	1:A:158:VAL:HG22	2.16	0.46
1:A:24:THR:O	1:A:28:LYS:HG3	2.16	0.46
1:B:341:ILE:CG2	1:B:342:VAL:N	2.79	0.46
1:B:346:ALA:O	1:B:350:VAL:HG23	2.16	0.46
1:B:38:LEU:C	1:B:40:ILE:N	2.69	0.46
1:B:113:PRO:O	1:B:116:LEU:N	2.49	0.45
1:B:188:PRO:HB2	1:B:220:GLU:HB3	1.99	0.45
1:B:95:ARG:HG2	1:B:95:ARG:NH1	2.30	0.45
1:A:173:HIS:ND1	1:A:206:ASN:OD1	2.42	0.45
1:A:238:PRO:HB3	1:A:247:TYR:CE1	2.51	0.45
1:B:18:LEU:HD12	1:B:60:VAL:O	2.17	0.45
1:B:81:LYS:O	1:B:85:ILE:HG13	2.17	0.45
1:A:402:ARG:HG2	1:A:430:TYR:CZ	2.51	0.45
1:B:1:MET:CA	2:B:580:HOH:O	2.64	0.45
1:B:208:SER:N	1:B:234:ASN:HD21	2.15	0.45
1:B:420:LEU:O	1:B:423:LYS:N	2.48	0.45
1:B:34:LEU:HD11	1:B:76:HIS:HD2	1.82	0.45
1:A:367:ILE:HD13	1:A:368:ASP:N	2.31	0.45
1:B:145:PHE:HZ	1:B:161:ALA:HB2	1.82	0.45
1:A:230:VAL:HG22	1:A:268:ILE:HB	1.98	0.45
1:B:260:SER:HA	1:B:263:GLU:HG3	1.98	0.45
1:A:457:ALA:O	1:A:461:LEU:HG	2.16	0.45
1:B:416:ASP:O	1:B:417:GLU:C	2.56	0.45
1:A:249:LEU:HD23	1:A:254:PHE:CD2	2.51	0.44
1:A:531:GLY:O	1:A:532:LEU:C	2.55	0.44
1:B:29:TYR:CD2	1:B:29:TYR:N	2.84	0.44
1:B:479:LEU:CD2	1:B:479:LEU:N	2.80	0.44
1:A:409:LEU:CD2	1:A:435:ILE:HG13	2.47	0.44
1:B:397:THR:O	1:B:400:ALA:HB3	2.16	0.44
1:A:71:MET:SD	1:A:109:THR:HG21	2.57	0.44
1:A:51:ARG:O	1:A:55:GLU:HG3	2.18	0.44
1:B:324:PRO:HG2	1:B:362:GLY:H	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:ARG:HB2	2:B:574:HOH:O	2.17	0.44
1:A:445:LYS:HE3	1:A:449:GLU:OE2	2.18	0.44
1:B:506:LEU:HA	1:B:506:LEU:HD12	1.86	0.44
1:B:73:LEU:HD22	1:B:78:LEU:HB2	1.99	0.44
1:B:255:ALA:HB2	1:B:282:LEU:HD22	1.98	0.44
1:B:282:LEU:HD23	1:B:286:VAL:HG23	2.00	0.44
1:A:188:PRO:HG3	1:A:217:ILE:HG23	1.99	0.44
1:B:145:PHE:CD2	1:B:157:ALA:HB1	2.52	0.44
1:B:180:GLY:O	1:B:181:ARG:HG2	2.16	0.44
1:B:235:ALA:HB3	1:B:247:TYR:HB3	2.00	0.44
1:B:282:LEU:CD2	1:B:286:VAL:HG23	2.48	0.44
1:B:70:ARG:NH2	1:B:70:ARG:CG	2.79	0.44
1:A:44:ASP:N	1:A:44:ASP:OD2	2.51	0.44
1:A:524:LEU:HD21	1:A:548:LEU:HG	1.99	0.44
1:B:145:PHE:CE2	1:B:157:ALA:HB1	2.53	0.44
1:A:236:GLY:HA3	1:A:249:LEU:HB2	2.01	0.43
1:A:76:HIS:N	1:A:76:HIS:ND1	2.66	0.43
1:A:258:ILE:N	1:A:258:ILE:HD12	2.33	0.43
1:B:177:ASP:OD1	1:B:179:LYS:N	2.51	0.43
1:B:324:PRO:HD3	1:B:360:ASN:O	2.18	0.43
1:B:75:LYS:C	1:B:76:HIS:ND1	2.71	0.43
1:A:125:TYR:C	1:A:125:TYR:CD1	2.91	0.43
1:A:340:GLU:HA	1:A:340:GLU:OE2	2.18	0.43
1:B:24:THR:HG22	1:B:28:LYS:HE3	2.01	0.43
1:B:441:LYS:HE3	1:B:453:TYR:CE2	2.52	0.43
1:B:61:ILE:CD1	1:B:97:ALA:HB2	2.48	0.43
1:A:369:VAL:HG12	2:A:628:HOH:O	2.18	0.43
1:B:207:CYS:O	1:B:208:SER:HB2	2.18	0.43
1:B:45:VAL:O	1:B:49:VAL:HG23	2.19	0.43
1:A:209:LEU:HD12	1:A:214:ILE:HD13	2.00	0.43
1:A:322:ILE:HG21	1:A:359:VAL:HG13	2.00	0.43
1:A:323:ASN:ND2	1:A:325:ALA:HB3	2.34	0.43
1:A:410:PHE:CE2	1:A:423:LYS:HD2	2.53	0.43
1:B:347:LYS:O	1:B:351:GLU:HG3	2.17	0.43
1:A:561:PRO:O	1:A:562:ARG:CB	2.67	0.43
1:B:1:MET:HA	2:B:580:HOH:O	2.17	0.43
1:B:484:LYS:N	1:B:485:PRO:CD	2.82	0.43
1:B:154:LEU:O	1:B:158:VAL:HG22	2.19	0.43
1:B:174:MET:HG3	1:B:191:PHE:CE1	2.53	0.43
1:B:255:ALA:HB1	1:B:286:VAL:HG21	2.00	0.43
1:A:154:LEU:HG	1:A:195:PHE:CE2	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:GLU:O	1:B:402:ARG:HG2	2.18	0.43
1:A:248:PRO:O	1:A:249:LEU:C	2.56	0.43
1:B:340:GLU:O	1:B:344:LYS:HB2	2.19	0.43
1:B:420:LEU:HD22	1:B:424:ILE:HD11	2.01	0.43
1:B:463:ARG:HD3	2:B:635:HOH:O	2.19	0.43
1:B:199:ASP:CG	1:B:199:ASP:O	2.55	0.43
1:B:219:GLN:HG2	1:B:223:GLN:HE21	1.84	0.43
1:A:339:GLU:O	1:A:343:ILE:HG13	2.19	0.42
1:B:493:GLU:HB2	1:B:530:LYS:HD2	2.00	0.42
1:B:422:MET:CE	1:B:426:LEU:HD12	2.48	0.42
1:B:537:MET:CE	1:B:548:LEU:HD22	2.48	0.42
1:A:234:ASN:OD1	1:A:273:CYS:HB2	2.18	0.42
1:A:325:ALA:HB2	1:A:360:ASN:HD21	1.84	0.42
1:A:443:VAL:HG11	1:A:477:LEU:HD11	2.01	0.42
1:A:26:PHE:CE1	1:A:49:VAL:HG21	2.54	0.42
1:A:532:LEU:HD11	1:A:534:SER:O	2.18	0.42
1:A:541:ASP:CG	1:A:544:LEU:HB2	2.39	0.42
1:B:386:PRO:HA	1:B:404:TYR:OH	2.20	0.42
1:A:162:ARG:HA	1:A:162:ARG:HD3	1.85	0.42
1:A:175:THR:HG23	1:A:175:THR:O	2.19	0.42
1:A:437:LEU:HG	1:A:439:MET:HG2	2.01	0.42
1:B:149:SER:HB3	1:B:183:LEU:CB	2.49	0.42
1:B:251:PRO:C	1:B:282:LEU:HD13	2.39	0.42
1:B:479:LEU:O	1:B:481:ALA:N	2.51	0.42
1:B:488:VAL:O	1:B:491:THR:N	2.52	0.42
1:A:503:THR:HA	1:A:534:SER:O	2.19	0.42
1:B:540:LEU:CD1	1:B:540:LEU:N	2.82	0.42
1:A:266:VAL:HG22	1:A:267:ASN:H	1.85	0.42
1:B:257:HIS:O	1:B:258:ILE:C	2.57	0.42
1:B:451:LYS:HG3	1:B:494:PHE:CE2	2.54	0.42
1:B:151:ILE:O	1:B:155:LYS:HB2	2.20	0.42
1:B:38:LEU:C	1:B:40:ILE:H	2.23	0.42
1:B:420:LEU:HA	1:B:420:LEU:HD23	1.91	0.42
1:A:255:ALA:HA	1:A:258:ILE:HD13	2.00	0.42
1:B:247:TYR:O	1:B:248:PRO:O	2.38	0.42
1:B:411:ASN:O	1:B:412:SER:HB3	2.20	0.42
1:B:255:ALA:HA	1:B:258:ILE:HD13	2.02	0.42
1:B:263:GLU:HG2	1:B:263:GLU:H	1.48	0.42
1:A:445:LYS:HB3	2:A:605:HOH:O	2.20	0.42
1:A:479:LEU:HD12	1:A:513:LEU:HD11	2.01	0.42
1:A:82:LEU:HD22	1:A:82:LEU:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LYS:C	1:B:29:TYR:HD2	2.23	0.42
1:B:393:ASN:HD22	1:B:396:LEU:HB2	1.85	0.42
1:B:132:VAL:HG13	1:B:143:ILE:HD13	1.99	0.41
1:B:330:LEU:C	1:B:332:ALA:N	2.73	0.41
1:B:321:ARG:HB3	1:B:345:GLU:OE2	2.20	0.41
1:B:388:SER:HA	1:B:409:LEU:O	2.19	0.41
1:A:295:ARG:O	1:A:296:LYS:O	2.37	0.41
1:B:10:LEU:O	1:B:10:LEU:HD12	2.20	0.41
1:B:53:TYR:CD2	1:B:280:VAL:HG21	2.56	0.41
1:A:162:ARG:CZ	1:A:170:LEU:HD12	2.50	0.41
1:B:162:ARG:HA	1:B:162:ARG:HD3	1.78	0.41
1:B:375:ILE:HA	1:B:375:ILE:HD13	1.88	0.41
1:A:249:LEU:HD23	1:A:254:PHE:CG	2.55	0.41
1:A:258:ILE:H	1:A:258:ILE:HD12	1.85	0.41
1:B:81:LYS:HD3	1:B:81:LYS:HA	1.78	0.41
1:A:279:HIS:HB3	1:A:283:PHE:CZ	2.54	0.41
1:A:562:ARG:CA	1:A:562:ARG:NE	2.81	0.41
1:B:11:LEU:HD12	1:B:11:LEU:HA	1.96	0.41
1:B:321:ARG:NH1	1:B:538:ASN:HB2	2.35	0.41
1:A:145:PHE:O	1:A:173:HIS:HB2	2.21	0.41
1:A:255:ALA:HA	1:A:258:ILE:CD1	2.50	0.41
1:A:1:MET:O	1:A:2:ARG:HB2	2.20	0.41
1:B:324:PRO:HG3	1:B:334:MET:CE	2.51	0.41
1:B:26:PHE:CE1	1:B:49:VAL:HG21	2.56	0.41
1:B:255:ALA:HA	1:B:258:ILE:CD1	2.50	0.41
1:B:463:ARG:HD2	2:B:613:HOH:O	2.20	0.41
1:A:200:ILE:HD11	1:A:203:LEU:HD21	2.03	0.41
1:A:152:LEU:CD2	1:A:377:GLN:HG3	2.50	0.41
1:B:443:VAL:HG12	1:B:443:VAL:O	2.21	0.41
1:B:59:ASP:HA	1:B:100:LYS:HG3	2.02	0.41
1:B:262:TYR:CZ	1:B:293:LEU:HD13	2.56	0.41
1:B:409:LEU:HD11	1:B:435:ILE:CD1	2.51	0.41
1:B:439:MET:CG	1:B:443:VAL:HG22	2.51	0.41
1:B:73:LEU:HD22	1:B:78:LEU:CB	2.51	0.41
1:A:282:LEU:O	1:A:283:PHE:C	2.59	0.41
1:B:262:TYR:HA	1:B:266:VAL:HG12	2.02	0.41
1:A:18:LEU:HB2	1:A:270:GLY:HA3	2.02	0.41
1:A:240:VAL:HB	1:A:243:GLY:CA	2.51	0.41
1:A:28:LYS:NZ	2:A:665:HOH:O	2.44	0.41
1:A:501:ASN:HD22	1:A:501:ASN:HA	1.54	0.41
1:B:369:VAL:O	1:B:369:VAL:HG12	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ARG:HG3	2:A:635:HOH:O	2.20	0.40
1:B:329:LYS:HA	1:B:329:LYS:HD2	1.91	0.40
1:B:361:PHE:CE1	1:B:372:VAL:HG13	2.56	0.40
1:B:40:ILE:HD13	1:B:88:ASN:ND2	2.36	0.40
1:A:123:GLU:HB2	2:A:618:HOH:O	2.20	0.40
1:A:391:ILE:CG2	1:A:396:LEU:HB3	2.51	0.40
1:A:540:LEU:N	1:A:540:LEU:HD12	2.36	0.40
1:A:76:HIS:O	1:A:78:LEU:HG	2.22	0.40
1:A:83:ASP:HB3	1:A:84:PRO:CD	2.51	0.40
1:B:272:CYS:HB3	1:B:273:CYS:H	1.55	0.40
1:B:345:GLU:O	1:B:349:GLN:HG3	2.21	0.40
1:B:404:TYR:CE1	1:B:408:SER:HB3	2.56	0.40
1:B:51:ARG:HH11	1:B:51:ARG:HG2	1.85	0.40
1:B:83:ASP:N	1:B:84:PRO:CD	2.84	0.40
1:B:193:ILE:HD11	1:B:300:ILE:HD11	2.03	0.40
1:A:181:ARG:HD2	1:A:185:GLY:O	2.20	0.40
1:A:539:PRO:HG2	1:A:540:LEU:CD1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	563/566 (100%)	490 (87%)	61 (11%)	12 (2%)	7	30
1	B	548/566 (97%)	462 (84%)	69 (13%)	17 (3%)	4	23
All	All	1111/1132 (98%)	952 (86%)	130 (12%)	29 (3%)	5	26

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	413	ALA
1	B	238	PRO
1	B	244	LYS
1	B	248	PRO
1	B	417	GLU
1	B	443	VAL
1	B	444	PRO
1	B	481	ALA
1	A	296	LYS
1	A	438	LEU
1	A	481	ALA
1	A	562	ARG
1	B	239	ILE
1	B	249	LEU
1	B	441	LYS
1	A	2	ARG
1	A	199	ASP
1	B	227	LYS
1	A	295	ARG
1	B	324	PRO
1	B	420	LEU
1	A	79	GLU
1	A	322	ILE
1	A	465	ASP
1	B	421	GLU
1	B	439	MET
1	B	542	GLU
1	B	35	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	492/494 (100%)	456 (93%)	36 (7%)	14	43
1	B	482/494 (98%)	445 (92%)	37 (8%)	13	41
All	All	974/988 (99%)	901 (92%)	73 (8%)	13	42

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	45	VAL
1	A	76	HIS
1	A	82	LEU
1	A	106	ILE
1	A	123	GLU
1	A	129	ARG
1	A	144	ILE
1	A	163	GLU
1	A	166	ARG
1	A	223	GLN
1	A	249	LEU
1	A	254	PHE
1	A	272	CYS
1	A	278	GLU
1	A	284	ARG
1	A	296	LYS
1	A	299	ARG
1	A	305	SER
1	A	323	ASN
1	A	360	ASN
1	A	367	ILE
1	A	370	ARG
1	A	396	LEU
1	A	409	LEU
1	A	445	LYS
1	A	458	LEU
1	A	459	LYS
1	A	463	ARG
1	A	501	ASN
1	A	506	LEU
1	A	509	LEU
1	A	513	LEU
1	A	548	LEU
1	A	558	LYS
1	A	562	ARG
1	B	2	ARG
1	B	34	LEU
1	B	48	LYS
1	B	61	ILE
1	B	70	ARG
1	B	94	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	151	ILE
1	B	152	LEU
1	B	163	GLU
1	B	178	GLU
1	B	198	LEU
1	B	200	ILE
1	B	207	CYS
1	B	217	ILE
1	B	238	PRO
1	B	244	LYS
1	B	249	LEU
1	B	254	PHE
1	B	256	VAL
1	B	263	GLU
1	B	272	CYS
1	B	278	GLU
1	B	285	LYS
1	B	296	LYS
1	B	320	GLU
1	B	392	GLN
1	B	399	ARG
1	B	422	MET
1	B	442	ASP
1	B	444	PRO
1	B	448	GLU
1	B	471	ILE
1	B	479	LEU
1	B	509	LEU
1	B	516	ARG
1	B	537	MET
1	B	554	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	323	ASN
1	A	335	GLN
1	A	520	ASN
1	B	338	ASN
1	B	393	ASN
1	B	425	ASN
1	B	508	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	565/566 (99%)	-0.42	7 (1%) 79 61	30, 51, 85, 100	0
1	B	552/566 (97%)	-0.40	4 (0%) 87 75	29, 49, 81, 100	0
All	All	1117/1132 (98%)	-0.41	11 (0%) 82 67	29, 50, 82, 100	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	GLY	4.7
1	A	241	GLU	2.9
1	A	561	PRO	2.9
1	A	242	ASN	2.7
1	B	242	ASN	2.6
1	A	240	VAL	2.5
1	A	563	ALA	2.4
1	B	241	GLU	2.4
1	B	30	GLY	2.3
1	B	245	THR	2.1
1	A	244	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.